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Theoretical studies of electric quadrupole transition probabilities in Mg II

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Abstract. The relativistic coupled cluster theory is employed to calculate electric quadrupole (E2) transition probabilities among the doublet states of Mg II which are of interest in astrophysical problems. This is the first time a highly correlated fully *ab initio* method has been used to compute these quantities for this particular ion. The line strengths and transition probabilities of a number of different transitions are reported and compared with those available in the literature.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding

1 Introduction

Forbidden radiative decays are generally observed only in low density regions between astronomical objects and in laboratory tokamak plasmas, where collisional deexcitation of metastable states is rather rare, leading to an accumulation of electrons in that level. These forbidden transitions can be used to obtain information about plasma temperature and dynamics [1]. Furthermore, the requirement for the medium to be of low density becomes less critical with highly ionized atoms of relatively high Z [2]. Electric quadrupole interactions are among the few important sources of hyperfine structure in atomic spectra. Transition lines of alkali-like atomic ions are important in astronomical observations as well as in laser cooling. For example, radiation of 2796 Å wavelength has been used in laser cooling setups for Mg II [3]. The basic theory of electric quadrupole (E2) radiation was given by Condon and Shortley [4]. Some of the methods used by Shortley could not be applied readily readily to more complicated atoms, and for this purpose Garstang [5,6] reformulated the theory of electric quadrupole interactions using the methods developed by Racah [7,8].

The combination of high spectral resolution, photometric precision and sensitivity, which come along with the latest generation of spectrographs, has motivated the study of UV interstellar absorption lines. This study enables a detailed examination of individual absorption regions in the interstellar medium (ISM). The strong near-UV Mg II lines are generally highly saturated along most interstellar lines outside the local ISM and usually yield extremely uncertain estimates of Mg II column densities in interstellar gas. Since Mg is predominantly in the singly ionized form in the neutral ISM *i.e.*, H I gas, and since Mg is expected to be a significant constituent of interstellar dust grains, the far-UV lines are critical for assessing the role of this important element in the ISM.

Forbidden emission lines of Mg II from the metastable levels are important as they are abundant in Solar flares [9]. Because of the relatively longer wavelengths of some E2 transitions, compared to wavelengths of the allowed transitions in the same ion, they can provide information on the thermal Doppler effect. The extreme ultraviolet (EUV) solar spectrum in the several hundred angstroms wavelength region provides a direct access to the physical conditions in the outer layers of the solar atmosphere from the chromosphere to the high temperature domain of the inner corona [10].

Spectroscopists have been looking for forbidden $3^2\mathrm{S}_{1/2}$–$n^2\mathrm{D}_{3/2,5/2}$ transitions in astrophysical objects since 1916 [11]. Accurate calculations of the rates of these transitions are a challenge to atomic theorists. Unlike neutral sodium, these transitions of Mg II corresponding to the same principal quantum number do not seem to have been observed in the laboratory, probably because the line is expected to be stronger than the Na I lines and so it may be more difficult to observe in experiments. Therefore, it is very likely that they may be present in the solar spectrum in emission [12]. Sandlin *et al.* [13] had observed few unidentified lines which are close to these transition lines. Also transitions to upper levels, *i.e.*, higher n values are interesting, particularly in the presence of electric fields.

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The first computation of the electric quadrupole transitions for Mg II was carried out by Warner [14] who had taken into account the spin-orbit interaction. Tull *et al.* [15] had used frozen core Hartree-Fock (HF) orbitals for the evaluation of these forbidden lines. A nonrelativistic model potential approach was used by Black *et al.* [16] to calculate the $3d(^2\mathrm{D})-3s(^2\mathrm{S})$ transition probability of Mg II. Our recent calculations [17] on allowed transitions of Mg II system has shown that the relativistic coupled cluster approach is a suitable method for computing highly accurate excitation energies and wavefunctions of the states. We have used this approach in the present work to calculate a large number of excitation energies and transition rates for Mg+. These data supersede earlier calculations that were carried out over three decades ago [14–16].

2 Theory

We start with a N-electron closed shell Dirac-Fock (DF) reference state $|\Phi\rangle$ and write the corresponding correlated closed shell state as

$$|\Psi\rangle = \mathrm{e}^T|\Phi\rangle \tag{1}$$

where T is the core electron excitation operator. In the present context, $|\Psi\rangle$ corresponds to the correlated ground state of Mg^{++} system. The Dirac-Coulomb equation

$$H\mathrm{e}^T|\Phi\rangle = E\mathrm{e}^T|\Phi\rangle \tag{2}$$

with

$$H = \sum_i c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)mc^2 + V_N + \sum_{i<j} \frac{1}{r_{ij}}$$

leads to the exact ground state energy E of closed shell part of the system. Here α and β are Dirac matrices and V_N is the nuclear potential. However, it is technically simpler to transcribe H in the occupancy number representation and use only the positive energy part of the orbital spectrum. Using the DF state $|\Phi\rangle$ with the lowest positive energy states occupied as the Fermi vacuum, it is convenient to define the normal ordered Hamiltonian

$$\tilde{H} \equiv H - \langle\Phi|H|\Phi\rangle = H - E_{DF}, \tag{3}$$

where $E_{DF} = \langle\Phi|H|\Phi\rangle$ and then solve the modified Dirac-Coulomb equation

$$\tilde{H}\mathrm{e}^T|\Phi\rangle = (E - E_{DF})\mathrm{e}^T|\Phi\rangle \equiv E_{\mathrm{corr}}\mathrm{e}^T|\Phi\rangle. \tag{4}$$

The Dirac-Coulomb Hamiltonian can also be written by explicitly including the positive energy projection operators [18]. However, Mittleman has shown that the Hamiltonian we have defined above implicitly contains these projection operators if we restrict our calculation to the space defined by the positive energy orbitals [19].

After projecting with $\langle\Phi|\mathrm{e}^{-T}$ from the left we obtain the correlation energy

$$\langle\Phi|\bar{H}|\Phi\rangle = E_{\mathrm{corr}}, \tag{5}$$

where we have defined the dressed, normal ordered Hamiltonian

$$\bar{H} = \mathrm{e}^{-T}\tilde{H}\mathrm{e}^T. \tag{6}$$

If we project any of the excited determinants $\langle\Phi^*|\mathrm{e}^{-T}$ from the left of equation (4) we additionally get the set of equations,

$$\langle\Phi^*|\bar{H}|\Phi\rangle = 0. \tag{7}$$

Equations (5) and (7) are the coupled cluster equations. First, the set of equation (7) has to be solved to yield the cluster operator T, which then can be used to define the dressed Hamiltonian $\bar{H}$ and to evaluate the correlation energy E_{corr}. In the CCSD (coupled cluster singles and doubles) approximation, the cluster operator T is composed of one- and two-body excitation operators, *i.e.*, $T = T_1 + T_2$, which are expressed in terms of second quantization,

$$T = T_1 + T_2 = \sum_{ap} a_p^+ a_a t_a^p + \sum_{abpq} a_p^+ a_q^+ a_b a_a t_{ab}^{pq}$$

After the contraction of the ladder operators [20] and rearranging the indices, equation (7) can be expressed in the following matrix form:

$$A + B(T) \cdot T = 0, \tag{8}$$

where A is a constant vector which consists of the elements $\langle\Phi^*|\tilde{H}|\Phi\rangle$ and the matrix $B(T)$ itself depends on the cluster amplitude so that equation (8) has to solved in a self-consistent manner.

Because of the spherical symmetry of atoms, the above derived equations can be separated into a radial and an angular part, which greatly simplifies the computational complexity of both DF and post-DF calculations. The corresponding angular factors can be derived by applying the graphical method of the angular momentum adaptation scheme [21], popularly known as the JLV [22]. The multi-pole expansion of the Coulomb operator is given in many text books [23–25]. Similarly, in the $|jm\rangle$ basis, the one- and two-body cluster operator T_1 and T_2 can be expressed as

$$t_a^p = \langle p|T_1|a\rangle = \sum_{j_a m_a} T_1^0(p,a)\delta(j_a,j_p)\delta(m_a,m_p) \tag{9}$$

and

$$\begin{aligned} t_{ab}^{pq} &= \langle pq|T_2|ab\rangle \\ &= \sum_{\begin{pmatrix} k, j_a m_a j_p m_p \\ j_b m_b j_q m_q \end{pmatrix}} T_2^k(p,q,a,b)(-1)^{(j_p - m_p + j_q - m_q)} \\ &\quad \times \begin{pmatrix} j_p & k & j_a \\ -m_p & q & m_a \end{pmatrix} \begin{pmatrix} j_q & k & j_b \\ -m_q & q & m_b \end{pmatrix} \cdot \end{aligned} \tag{10}$$

Here, $T_2^k(p,q,a,b)$ denotes the radial cluster operator, depending on the multi-pole k, the orbital indices a,b (occupied orbitals) and p,q (virtual orbitals), which is multiplied by a phase factor and the appropriate Wigner $3j$-symbols. Applying the multi-pole expansion of the

Coulomb operator and the cluster operator T together with the JLV scheme, the angular momentum reduction of the CC equations is straightforward. For the angular part of the Coulomb matrix element we can derive the constraints

$$(-1)^{l_a+l_c+k} = 1 \ \text{ and } \ (-1)^{l_b+l_d+k} = 1. \tag{11}$$

The above constraints have to be satisfied only in the CC diagrams which contain the Coulomb integrations in less than third order (*i.e.* during the first iteration; then the cluster operator itself represents one order in Coulomb interaction), whereas higher order Coulomb interactions (in later iterations) lead to coupled angular momenta which violate equation (11). The excitations, which satisfy equation (11), are called *even-parity pair channels* (EPC). Liu *et al.* [26] have argued that the EPC provide the dominant contribution to the CC equations and therefore it might be a valid approximation to discard the odd-parity pair channels (OPC) and in this way the number of cluster amplitudes and the computational effort reduces by a factor of half. We have followed this suggestion and applied the CC approach to only EPC cluster amplitudes, which we shall refer to as the CCSD-EPC approximation.

The ground state of Mg^+ contains only one valence electron in the $3s_{1/2}$ orbital. One way to evaluate the ground state energy of Mg^+ is to first compute the correlations within the closed shell system Mg^{++} using the closed shell CC approach and then add another electron to the $3s_{1/2}$ orbital with the help of the open shell CC (OSCC) technique [27]. Similarly, the valence electron can be added to any other orbital to yield excitation energies. In order to add an electron to the kth virtual orbital of the DF reference state we define

$$|\Phi_k^{n+1}\rangle \equiv a_k^\dagger|\Phi\rangle \tag{12}$$

with the particle creation operator $a_k^\dagger$. We now define the exact state using excitation operators for both, the core electrons and the valence electron, in the following way:

$$|\Psi_k^{n+1}\rangle = \mathrm{e}^T\{\mathrm{e}^{S_k}\}|\Phi_k^{n+1}\rangle \tag{13}$$

where $\{\mathrm{e}^{S_k}\}$ is the normal ordered exponential representing the valence part of the wave-operator [25]. S_k itself is also in normal order and both are normal ordered with respect to $|\Phi\rangle$. Since S_k has to contain the particle annihilation operator a_k, because of the normal ordering it cannot be connected to any other valence electron excitation operator so that $\{\mathrm{e}^{S_k}\}$ reduces to $(1+S_k)$ and we can write equation (13) as

$$|\Psi_k^{n+1}\rangle = \mathrm{e}^T(1+S_k)|\Phi_k^{n+1}\rangle. \tag{14}$$

Following the same procedure as in the closed shell approach, we obtain a set of equations

$$\langle\Phi_k^{n+1}|\bar{H}(1+S_k)|\Phi_k^{n+1}\rangle = \Delta E_k, \tag{15}$$

and

$$\langle\Phi_k^{*,n+1}|\bar{H}(1+S_k)|\Phi_k^{n+1}\rangle = \Delta E_k\langle\Phi_k^{*,n+1}|S_k|\Phi_k^{n+1}\rangle. \tag{16}$$

Here, ΔE_k is the difference between the energy of the single reference state $|\Psi_k^{n+1}\rangle$ and the closed shell state $|\Psi\rangle$. (The operators in left hand side of Eq. (15) and both sides of Eq. (16) are connected). Equation (16) is nonlinear in S_k because the energy difference ΔE_k itself is a function of S_k. These equations have to be solved self-consistently to determine the S_k-amplitudes [28].

The next step in the calculation is the inclusion of the triple excitations in an approximate way using

$$S_{abk}^{pqr} = \frac{\widehat{VT_2} + \widehat{VS_2}}{\epsilon_a + \epsilon_b + \epsilon_k - \epsilon_p - \epsilon_q - \epsilon_r} \tag{17}$$

where S_{abk}^{pqr} are the amplitudes corresponding to the simultaneous excitation of orbitals a, b, k to p, q, r; $\widehat{VT}$, $\widehat{VS}$ are the correlated composites involving V and T, and V and S respectively. ϵ_i is the orbital energy of the ith orbital. This contribution is added to the energy obtained using singles and doubles.

The definition of the line strength in atomic unit $(e^2a_\mathrm{o}^4)$ of a electric quadrupole transition from $|\Psi_i\rangle$ to $|\Psi_f\rangle$ is

$$\begin{aligned} S_{fi} &= |\mathbf{Q}_{fi}|^2 \\ &= \sum_{m_f,m_i} |\langle\Psi_f|\mathbf{Q}|\Psi_i\rangle|^2 \\ &= \sum_{m_f,m_i}\sum_q (2J_f+1)\begin{pmatrix} j_f & 2 & j_i \\ -m_f & q & m_i \end{pmatrix}^2 |\langle\Psi_f||\mathbf{Q}||\Psi_i\rangle|^2 \\ &= \sum_q \frac{(2J_f+1)}{5}|\langle\Psi_f||C^2r^2||\Psi_i\rangle|^2 \\ &= (2J_f+1)\langle\chi_f||C^2||\chi_i\rangle^2|\langle R_f|r^2|R_i\rangle|^2 \\ &= (2J_f+1)(2J_i+1)\begin{pmatrix} j_f & 2 & j_i \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}^2 |\langle R_f|r^2|R_i\rangle|^2 \end{aligned} \tag{18}$$

where χ_f and χ_i are the angular part of the final and initial states, and R_f and R_i are the radial part of the final and initial states.

In our case the initial and final states are not normalized. Therefore,

$$\mathbf{Q}_{fi} = \frac{\langle\Psi_f|\mathbf{Q}|\Psi_i\rangle}{\sqrt{\langle\Psi_f|\Psi_f\rangle}\sqrt{\langle\Psi_i|\Psi_i\rangle}}, \tag{19}$$

where

$$\langle\Psi_f|\mathbf{Q}|\Psi_i\rangle = \langle\Phi_f^{n+1}|\{\mathrm{e}^{S_f^\dagger}\}\bar{Q}\{\mathrm{e}^{S_i}\}|\Phi_i^{n+1}\rangle. \tag{20}$$

$\bar{Q} = \mathrm{e}^{T^\dagger}Q\,\mathrm{e}^T$ and Q is the electric quadrupole moment operator as defined above. The connected parts of equation (19) and equation (20) will contribute and hence we only compute those parts in our quadrupole matrix element calculations.

$\bar{Q}$ gives rise to a non-terminating series and consequently the matrix element of Q given in equation (20) contains an infinite number of terms. It is indeed possible to express $\bar{Q}$ diagramtically in terms of uncontracted single particle lines The fully contracted part of this will

Transition	Multiplets	SO^a	HF^b	CCSD(T)
$3s \rightarrow 3d$	^{2}S$_{1/2}$–^{2}D$_{3/2}$	1.17×10^{-5}		0.887×10^{-5}
	^{2}S$_{1/2}$–^{2}D$_{5/2}$	1.77×10^{-5}		1.330×10^{-5}
	addition of the multiplets	2.94×10^{-5}	1.47×10^{-5}	2.227×10^{-5}
$3s \rightarrow 4d$	^{2}S$_{1/2}$–^{2}D$_{3/2}$	0.77×10^{-6}		0.685×10^{-6}
	^{2}S$_{1/2}$–^{2}D$_{5/2}$	1.47×10^{-6}		1.027×10^{-6}
	addition of the multiplets	2.24×10^{-6}	1.20×10^{-6}	1.712×10^{-6}

Table 1. Comparison of gf-value of E2 transitions of 3^2S to n^2D of Mg II; ^{a}: method using spin-orbit interaction [14], ^{b}: HF method [15].

not contribute as it cannot be linked with the remaining part of the expression. Terms with two uncontracted lines (one incoming and one outgoing) are called one-body terms and terms with four uncontracted lines (two incoming and two outgoing) are called two-body terms and so on. Finally, all these diagrams with uncontracted lines are made fully contracted with S-operators in order to express it in a form that can be readily computed. We have considered the contributions from the one and two-body terms in the present work as the three and higher-body terms can be argued to be very small [29].

The transition probability (in s^{-1}) of the electric quadrupole transition is related to the line strength by

$$g_i A_{if} = (1.119896 \times 10^{18}/\lambda^5)S. \tag{21}$$

3 Computations

The DF ground orbitals for Mg$^+$ were calculated using a novel approach discussed in our earlier papers [30, 31]. This approach uses the finite basis set expansion method (FBSE) in the framework of Gaussian-type orbitals (GTO) and the numerical orbitals obtained by running the GRASP code [32]. A large basis set of $(30s25p25d20f15g)$ Gaussian-type functions of the form

$$F_{i,k}(r) = r^k \mathrm{e}^{-\alpha_i r^2} \tag{22}$$

with $k = 0, 1, 2, ...$ for s, p, d, ..., respectively, is used to construct the FBSE. For the exponents, the universal even tempering condition

$$\alpha_i = \alpha_{i-1}\beta, \qquad i = 1, ..., N \tag{23}$$

was applied. Here, N is the number of basis functions for a specific symmetry. We have used $\alpha_\circ = 0.001$ and $\beta = 2.90$ for all symmetries.

The starting point of this calculation is the generation of DF orbitals for the Mg^{++} core, where orbitals were stored on a grid. Though we have used a large basis space for the generation of the orbitals, from our past experience [27] we restrict the number of basis orbitals for the coupled cluster calculation by imposing an upper bound in energy for all single particle orbitals of s-, $p_{1/2}$-, $p_{3/2}$-symmetries by 1500 a.u., $d_{3/2}$-, $d_{5/2}$-, $f_{5/2}$-, $f_{7/2}$-symmetries by 500 a.u. and $g_{7/2}$, $g_{9/2}$ symmetries by 5 a.u. This is done to reduce the huge memory required to store the matrix elements of the dressed operator $\bar{H}$ and the two electron coulomb interaction in the main memory. We have included all the singles, doubles and partial triple excitations from the core in the present calculations.

Table 2. Comparison of the line strength of E2 transitions among the states of same orbital quantum numbers of Mg II with the MCHF method.

Transition	Multiplets	MCHF	CCSD(T)
$3p \rightarrow 3p$	^{2}P$_{1/2}$–^{2}P$_{3/2}$	1.476×10^2	1.505×10^2
$3p \rightarrow 4p$	^{2}P$_{1/2}$–^{2}P$_{3/2}$	7.855×10^1	7.755×10^1
$3p \rightarrow 4p$	^{2}P$_{3/2}$–^{2}P$_{3/2}$	7.877×10^1	7.397×10^1
$3d \rightarrow 3d$	^{2}D$_{3/2}$–^{2}D$_{5/2}$	2.982×10^1	3.017×10^2
$3d \rightarrow 4d$	^{2}D$_{3/2}$–^{2}D$_{5/2}$	1.705×10^2	1.785×10^2
$4p \rightarrow 4p$	^{2}P$_{1/2}$–^{2}P$_{3/2}$	3.526×10^3	3.580×10^3
$4d \rightarrow 4d$	^{2}D$_{3/2}$–^{2}D$_{5/2}$	4.940×10^3	5.008×10^3

4 Results and discussions

The correlation effect is rather large for excitation energies of Mg$^+$ compared to heavier Na-like ions. Therefore, these correlations have to be computed very accurately in order to obtain high precision atomic data. We have used the relativistic coupled-cluster method in order to account for these large correlation effects. The reason for our choice of an *ab initio* relativistic method based on the Dirac-Coulomb Hamiltonian as discussed in Section 2 is to incorporate the relativistic effects more rigorously than Warner [14], who has considered spin-orbit effects in his work.

In our earlier work [17] we have shown that the relativistic coupled cluster method (CCSD(T)) produces very accurate excitation energies and electric dipole transition rates for Mg II, which resolved one of the long standing problem for this ion [34]. We have tested the accuracy of our wave functions by comparing electric dipole matrix elements for the length and velocity gauges. Therefore, one can expect that the same wavefunctions should also lead to accurate numbers for the E2 transition rates and improve earlier results obtained with the Hartree-Fock (HF) method [15] and other, non-relativistic methods based on model potentials [16]. Warner [14] has taken explicit account of the spin-orbit (SO) interaction in calculating his radial functions and obtained E2 transitions strength much larger than Hartree-Fock values [15]. In Table 1, we have made a comparison of different gf-values for 3^2S$_{1/2}$–n^2D$_{3/2,5/2}$ transitions with the earlier calculations. To compare with the HF results reported by Tull *et al.*, we have added the results of the multiplets and put them in a separate row. Our results lie between the values of other two results.

In Table 2, we have compared our calculated line strengths with unpublished work of Froese Fischer using

Table 3. Line strengths of E2 transitions of S to D multiplets for Mg II. [Note: in transition prob. column, A_{if} value calculated with NIST excitation energy value are given inside parenthesis.]

Transition	Multiplet	Wave length in Å	Line strength in a.u.	Transition prob. in s^{-1}
$3s \rightarrow 3d$	$^2S_{1/2}-^2D_{3/2}$	1398.77	0.96403×10^2	$5.010 \times 10^3 (5.040 \times 10^3)$
$4d$		1071.68	0.33479×10^1	$0.659 \times 10^3 (0.663 \times 10^3)$
$5d$		966.93	0.13453×10^1	$0.443 \times 10^3 (0.445 \times 10^3)$
$3s \rightarrow 3d$	$^2S_{1/2}-^2D_{5/2}$	1398.79	0.14461×10^3	$5.010 \times 10^3 (5.040 \times 10^3)$
$4d$		1071.69	0.50187×10^1	$0.658 \times 10^3 (0.662 \times 10^3)$
$5d$		966.934	0.20198×10^1	$0.443 \times 10^3 (0.446 \times 10^3)$
$4s \rightarrow 3d$	$^2S_{1/2}-^2D_{3/2}$	59308.1	0.90811×10^3	$0.342 \times 10^{-3} (0.346 \times 10^{-3})$
$4d$		4254.2	0.14646×10^4	$0.293 \times 10^3 (0.294 \times 10^3)$
$5d$		2974.8	0.10457×10^3	$0.125 \times 10^3 (0.125 \times 10^3)$
$4s \rightarrow 3d$	$^2S_{1/2}-^2D_{5/2}$	59338.7	0.13624×10^4	$0.342 \times 10^{-3} (0.346 \times 10^{-3})$
$4d$		4254.3	0.21965×10^4	$0.293 \times 10^3 (0.293 \times 10^3)$
$5d$		2974.9	0.15693×10^3	$0.125 \times 10^3 (0.126 \times 10^3)$
$5s \rightarrow 3d$	$^2S_{1/2}-^2D_{3/2}$	4694.9	0.12061×10^3	$0.147 \times 10^2 (0.148 \times 10^2)$
$4d$		192086.1	0.13541×10^5	$0.144 \times 10^{-5} (0.145 \times 10^{-4})$
$5d$		9407.8	0.11163×10^5	$0.422 \times 10^2 (0.424 \times 10^2)$
$5s \rightarrow 3d$	$^2S_{1/2}-^2D_{5/2}$	4694.8	0.18105×10^3	$0.148 \times 10^2 (0.148 \times 10^2)$
$4d$		192278.1	0.20314×10^5	$0.144 \times 10^{-4} (0.144 \times 10^{-4})$
$5d$		9408.0	0.16741×10^5	$0.422 \times 10^2 (0.424 \times 10^2)$

Table 4. Line strengths of E2 transitions of $P_{1/2}$ to $P_{3/2}$ multiplets for Mg II. [Note: in transition prob. column, A_{if} value calculated with NIST excitation energy value are given inside parenthesis.]

Transition	Multiplet	Wave length	Line strength	Transition prob.
$3p \rightarrow 3p$	$^2P_{1/2}-^2P_{3/2}$		0.15050×10^3	$0.305 \times 10^{-10} (0.271 \times 10^{-10})$
$4p$		2223.2	0.77549×10^2	$0.397 \times 10^3 (0.399 \times 10^3)$
$5p$		1618.1	0.57577×10^1	$0.144 \times 10^3 (0.145 \times 10^3)$
$4p \rightarrow 3p$	$^2P_{1/2}-^2P_{3/2}$	2229.2	0.78304×10^2	$0.790 \times 10^3 (0.796 \times 10^3)$
$4p$			0.35803×10^4	$0.296 \times 10^{-11} (0.266 \times 10^{-11})$
$5p$		5934.9	0.11751×10^4	$0.444 \times 10^2 (0.446 \times 10^2)$
$5p \rightarrow 3p$	$^2P_{1/2}-^2P_{3/2}$	1620.9	0.57595×10^1	$0.286 \times 10^3 (0.288 \times 10^3)$
$4p$		5950.6	0.11851×10^4	$0.884 \times 10^2 (0.889 \times 10^2)$
$5p$			0.33841×10^5	$0.535 \times 10^{-12} (0.473 \times 10^{-12})$
$3p \rightarrow 4p$	$^2P_{3/2}-^2P_{3/2}$	2227.7	0.73968×10^2	$0.375 \times 10^3 (0.377 \times 10^3)$
$5p$		1620.5	0.52204×10^1	$0.130 \times 10^3 (0.130 \times 10^3)$
$4p \rightarrow 5p$	$^2P_{3/2}-^2P_{3/2}$	5945.7	0.11035×10^4	$0.414 \times 10^2 (0.415 \times 10^2)$

multiconfiguration Hartree-Fock method (MCHF) with Breit-Pauli approximation [35] between states having same orbital quantum numbers (as, she has given only these number in her web-site) and do see good agreement with our results. The CC theory unlike the MCHF method is size-consistent [20]. Also CC theory incorporates certain important higher order excitations that the MCHF method does not at the same level of approximation. For example, CC singles and doubles includes not only T_2 but also T_2^2, but MCHF singles and doubles only has the effects of the former. T_2^2 terms in the MCHF method arise only when one considers quadrupole excitations.

In Table 3, we have presented our E2 transition results among the S–D doublet states. We have also used both the experimental and the computed excitation energies to calculate the transition probabilities. We observed a very good agreement among them, as our calculated excitation energies were already very accurate.

In Tables 4 and 6, we have presented results of our E2 transition calculations between states of same orbital angular momentums. Though the line strengths of E2 transitions between the states of same principal quantum numbers given in these tables are large, their transition probabilities are rather very small due to large wavelengths. They fall in the far infra-red region or beyond, and we have not put their wavelengths in the tables. Table 5, reports E2 transition results for different multiplets between ^2P to ^2F states.

Table 5. Line strengths of E2 transitions of P to F multiplets for Mg II.

Transition	Multiplet	Wave length	Line strength	Transition prob.
$3p \to 4f$	$^2\mathrm{P}_{1/2}$–$^2\mathrm{F}_{5/2}$	1720.3	0.21321×10^3	0.262×10^4
$5f$		1470.1	0.43542×10^2	0.117×10^4
$4p \to 4f$	$^2\mathrm{P}_{1/2}$–$^2\mathrm{F}_{5/2}$	7587.2	0.64512×10^4	0.473×10^2
$5f$		4334.6	0.39740×10^3	0.481×10^2
$5p \to 4f$	$^2\mathrm{P}_{1/2}$–$^2\mathrm{F}_{5/2}$	27356.1	0.58201×10^5	0.101×10^2
$5f$		16039.2	0.19724×10^4	0.116×10^4
$3p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{5/2}$	1722.9	0.61239×10^2	0.746×10^3
$5f$		1472.1	0.12422×10^2	0.333×10^3
$4p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{5/2}$	7604.8	0.18460×10^4	0.134×10^2
$5f$		4340.3	0.11430×10^3	0.137×10^2
$5p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{5/2}$	27120.1	0.21361×10^4	0.271×10^{-1}
$5f$		16121.4	0.16671×10^5	0.286×10^1
$3p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{7/2}$	1723.0	0.36743×10^3	0.336×10^4
$5f$		1472.1	0.74533×10^2	0.150×10^4
$4p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{7/2}$	7604.7	0.11076×10^5	0.602×10^2
$5f$		4340.3	0.68573×10^3	0.618×10^2
$5p \to 4f$	$^2\mathrm{P}_{3/2}$–$^2\mathrm{F}_{7/2}$	27121.1	0.12817×10^5	0.122×10^0
$5f$		16121.2	0.10003×10^6	0.129×10^2

Table 6. Line strengths of E2 transitions of $\mathrm{D}_{3/2}$ to $\mathrm{D}_{5/2}$ and $\mathrm{F}_{5/2}$ to $\mathrm{F}_{7/2}$ multiplets for Mg II.

Transition	Multiplet	Wave length	Line strength	Transition prob.
$3d \to 3d$	$^2\mathrm{D}_{3/2}$–$^2\mathrm{D}_{5/2}$		0.30174×10^3	0.138×10^{-21}
$4d$		4583.0	0.16857×10^3	0.155×10^2
$5d$		3131.98	0.83417×10^1	0.515×10^1
$4d \to 3d$	$^2\mathrm{D}_{3/2}$–$^2\mathrm{D}_{5/2}$	4582.75	0.16927×10^3	0.156×10^2
$4d$			0.50083×10^4	0.347×10^{-21}
$5d$		9892.6	0.17248×10^4	0.339×10^1
$5d \to 3d$	$^2\mathrm{D}_{3/2}$–$^2\mathrm{D}_{5/2}$	3131.86	0.83988×10^1	0.534×10^{-2}
$4d$		9891.77	0.17331×10^4	0.342×10^1
$5d$			0.37631×10^5	0.195×10^{-21}
$4f \to 4f$	$^2\mathrm{F}_{5/2}$–$^2\mathrm{F}_{7/2}$		0.18425×10^4	0.259×10^{-9}
$5f$		8458.29	0.79110×10^3	0.256×10^1
$5f \to 4f$	$^2\mathrm{F}_{5/2}$–$^2\mathrm{F}_{7/2}$	10214.4	0.78960×10^3	0.104×10^1

5 Conclusion

We have calculated accurate E2 transition probabilities for Mg II, which is important in astrophysics and laboratory plasma physics, using the *ab initio* all order relativistic coupled cluster method. The line strengths of some of the transitions which are presented in this work have, to our knowledge, not been calculated earlier. There is a need for such calculations due to the advent of high resolution spectrographs and the demand for high precision computations is likely to increase in the future.

A part of this work was done on the Beowulf cluster at the Harish-Chandra Research Institute:
`http://cluster.mri.ernet.in`.

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